SANDIA REPORT
SAND2007-0901
Unlimited Release
Printed April 2007

Atomistic Simulations of Brittle Crack Growth

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National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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Introduction

Ceramic materials such as lead zirconium titanates (PZT), low temperature co-fired ceramics and silica glasses are used in several of Sandia's mission critical components. Brittle fracture, either during machining and processing or after many years in service, remains a serious reliability and cost issue. Despite its technological importance, brittle fracture remains poorly understand, especially the onset and propagation of sub-critical cracks. However, some insights into the onset of fracture can be gleaned from the atomic scale structure of the amorphous material. In silica for example, it is well known [1] that the Si-O-Si bonds are relatively weak and, in angle distribution functions determined from scattering experiments, the bonds exhibit a wide spread around a peak at 150^o. By contrast the O-Si-O bonds are strong with a narrow peak in the distribution around the 109^o dictated by the SiO_4 tetrahedron. In addition, slow energy release in silica, as deduced from dissolution experiments, depends on the distribution of 3-fold and higher rings in the amorphous structure [2].

The purpose of this four month LDRD project was to investigate the atomic structure of silica in the bulk and in the vicinity of a crack tip using molecular dynamics simulations. Changes in the amorphous structure in the neighborhood of an atomically sharp tip may provide important clues as to the initiation sites and the stress intensity required to propagate a sub-critical crack.

Numerical Procedures

In this study silica was modeled using the interatomic potential developed by van Beest, Kramer and van Santen (BKS) [3]. In the BKS model the energy of interaction between atoms depends on three terms: a long range attractive contribution given by a Lennard-Jones form, ie. $1/r^6$, a short range repulsive part described by an exponential function and a Coulombic contribution where the charges are given by q_{Si}=2.4 and q_O=-1.2. All parameters of the potential were found by fitting to both ab-initio atomistic simulations and experimental data.

An amorphous silica structure was prepared by first melting a system consisting of 43845 atoms (135.8x80.7x104.1 A^3) at a temperature of 3000K for 200ps. The melting step employed an NPT ensemble with a time step of 1 fs and periodic boundary conditions were applied. In all simulations the code LAMMPS, developed at Sandia, was used. Subsequent to melting, the system was cooled from 3000K to room temperature (300K) in a 200 ps run.

An important consideration in the present work is introducing a crack in the silica surface while maintaining the correct stoichiometry. First, free surfaces were formed in the x direction, the left and right sides of Fig. 1, by extending the periodic bounds. Then, a triangular shaped crack was established by the following procedure. A crack opening length and a crack depth were, which

defines two sloped lines between which all silicon, but not oxygen, atoms are removed. As shown in Fig. 1 the center of the crack lies on the left surface of the system and is positioned half the distance along the y dimension. Then a new crack opening, 10% smaller than the initial value, was assumed, but the angle formed by the crack surface remained the same. The number of oxygen atoms within the smaller triangle was computed. The crack opening was then increased in small increments until the number of oxygen atoms equaled twice the number of Si atoms removed initially. The final crack formed by this procedure is shown in Fig. 1 where the red atoms are Si and the green denotes O.

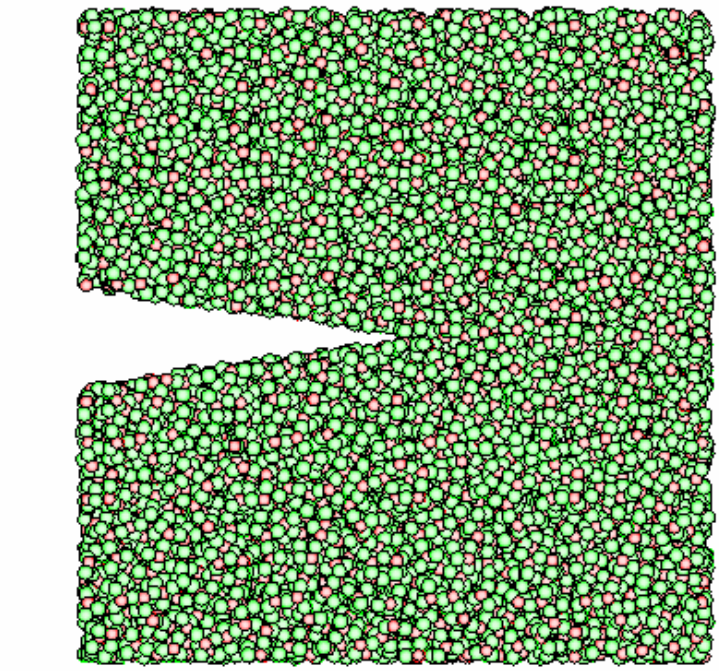

Figure 1. The silica system with a surface crack introduced. Red atoms represent Si and the green is oxygen.

Unfortunately, severe numerical problems were encountered when running MD simulations of the cracked silica system. It was observed that, even at short times, atoms were ejected from the free surfaces. A number of simulation parameters were varied in an effort to prevent the problem, but none proved successful. The time step was decreased to the very small .01 fs, a Fourier space, as well as a real space, Ewald summation technique was attempted and no Ewald sum was applied, but the cutoff range of the potential was increased to 10A.

Some success was found in a simpler system with no crack introduced. Atoms on both free surfaces that were undercoordinated, that is containing only one neighbor within a prescribed cutoff radius, were identified. Then, undercoordinated O atoms were moved to positions within the nearest neighbor distance of undercoordinated Si atoms. The scheme however, was only partially successful. The highly energetic, repositioned atoms remained on the surface during

MD simulations, but others were ejected from the system. Furthermore, with the crack introduced more atoms were observed to escape from the system.

Conclusions

Although MD simulations offer great promise in elucidated many important features of sub-critical crack growth, an additional numerical procedure is required for continued progress. A code should be developed which will correctly identify all the surface atoms that will be unstable in an MD simulation and rearrange them to positions of lower energy. The pre-processing scheme must be sufficiently robust to handle the case of atoms located at the surfaces of an atomistically sharp tip.

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